

Comment on “Zeeman-Driven Lifshitz Transition: A Model for the Experimentally Observed Fermi-Surface Reconstruction in YbRh₂Si₂”

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In Phys. Rev. Lett. 106, 137002 (2011), A. Hackl and M. Vojta have proposed to explain the quantum critical behavior of YbRh₂Si₂ in terms of a Zeeman-induced Lifshitz transition of an electronic band whose width is about 6 orders of magnitude smaller than that of conventional metals. Here, we note that the ultra-narrowness of the proposed band, as well as the proposed scenario *per se*, lead to properties which are qualitatively inconsistent with the salient features observed in YbRh₂Si₂ near its quantum critical point.

The field-induced transition out of an antiferromagnetic (AF) order in YbRh₂Si₂ has emerged as a prominent example of local Kondo-destruction quantum critical point (QCP) [1–3]. This class of QCP goes beyond the Landau framework of order-parameter fluctuations, involving a localization-delocalization transition of the f-electrons across the AF transition; the Fermi surface experiences a sudden jump from “small” (f-electrons being localized) to “large” (f-electrons delocalized) at zero temperature [4, 5]. In YbRh₂Si₂, the evolution of the Hall coefficient as a function of magnetic field provides the most direct evidence for such a Fermi-surface jump across a field-driven QCP [1, 2], which is corroborated by the evolutions of the magnetoresistivity [1, 2] and thermodynamic properties [3]. This jump in the Fermi surface across the AF critical field B_N , which is about 0.06 T for a field applied within the *ab* plane of the tetragonal crystalline structure, appears to be accompanied by the divergence of the quasiparticle mass [6].

In a recent paper [7], Hackl and Vojta (HV) proposed an alternative interpretation of these observations in YbRh₂Si₂ near B_N , based on a Lifshitz transition associated with the bandstructure of non-interacting electrons or weakly-interacting quasiparticles. HV postulated a hitherto unknown ultra-narrow band, with one component of its Zeeman-split Fermi surface shifting below (or above) the Fermi energy at the critical field. (In the standard classification of Lifshitz transitions, this belongs to the “void” type [8].) Because the critical field in this case is very small (in contrast to other cases of heavy fermions where a field-induced Lifshitz transitions have been implicated [9, 10]), HV had to assume an exceedingly small bandwidth of about 5 μ eV.

Here, we argue that the scenario of HV is unlikely to be pertinent to the physics near B_N in YbRh₂Si₂. A number of key features in the HV proposal contradict the salient experimental results.

A. Clearly, for a bandwidth of 5 μ eV invoked in the scenario of HV, temperatures above about 50 mK remove

the underlying Fermi surface and would therefore wash out the features of the Lifshitz transition in the isothermal Hall coefficient and magnetoresistivity. This is in contradiction to the experiment, in which the isothermal crossover can be traced up to about 20 times as high a temperature (about 1 K), as illustrated by Fig. 1a (Ref. [1]).

B. The 5 μ eV bandwidth is so small that it would lead to an entropy crisis.

B1. Considering that 5 μ eV is about 6 orders of magnitude smaller than the typical bandwidth of a simple metal, the scenario of HV would very generally yield a huge specific-heat coefficient, $\gamma \equiv C_{el}/T$. For example, the calculation reported in Fig. 3 of Ref. [7] is based on a full conduction-electron band (which has an entropy of the order of $R \ln 2$) of width about 5 μ eV. The corresponding γ will be about 10^3 J/mol \cdot K², which is 6 orders of magnitude larger than that of a simple metal. Compared to the value observed experimentally at around 50 mK (about 1 J/mol \cdot K²) [6], this is 3 orders of magnitude too large. Equivalently, while the experimental observation has established that the entropy associated with the quantum critical regime of YbRh₂Si₂, about 0.4 $R \ln 2$, is distributed in a temperature range of about 10K, the scenario of HV would spread a similarly large entropy over a temperature range of about 50 mK.

B2. In a separate calculation, reported in their Fig. 2, HV took the small-width band as riding on top of a background portion corresponding to quasiparticles with a Kondo scale of about 25 K. Because the invoked narrow band contains about 25% of the spectral weight of the full band, the involved entropy is still too large – 25% of $R \ln 2$ over a temperature range of 50 mK. The γ expected at around 50 mK will still be much (25% of three orders of magnitude) too large compared with the experimental observation. Thus, this does not resolve the above entropy crisis.

B3. These order-of-magnitude issues should not be taken as quantitative problems. Instead, they represent

qualitative discrepancies with the experiments that are inherent to the assumed ultra-low Fermi energy scale. The background density-of-states (DOS) is associated with the 25 K energy scale, which already corresponds to a γ of the order 1 J/mol · K². The proposed small peak of the DOS in the HV scenario can then only be of a similar height as the background one; in other words, it would hardly be a peak. Equivalently, its spectral weight must be so small (with the associated entropy on the order of 0.2% R ln 2) that it will hardly have any observable consequence.

C. We next turn to the specific critical behavior. A void Lifshitz transition, with the Fermi surface continuously shrinking to zero, will lead to only weak singularities in the resistivity and Hall effect as a function of the control parameter. In two dimensions, it typically yields a cusp in the Hall coefficient and a change in slope in the residual resistivity. In three dimensions, the features are even weaker. In the scenario of HV, therefore, the isothermal Hall coefficient and magnetoresistivity will both remain continuous across the Zeeman-induced Lifshitz transition down to $T = 0$. Experimentally, however, both quantities in YbRh₂Si₂ have been shown to jump in the extrapolated $T = 0$ limit: they exhibit a crossover from one constant to another at $B^*(T)$, and the crossover width Γ goes to zero in the $T = 0$ limit. It should be stressed that, while experimental measurements are of course done at finite temperatures, our extrapolation of Γ to the $T = 0$ limit is based on the observation that it is proportional to T for more than 1.5 decades of temperature as shown in Fig. 1a [1].

D. Because the void Lifshitz transition simply involves a continuous shrinking of a Fermi pocket, it will produce neither a maximum nor a divergence of the effective mass at the transition point. Indeed, in HV's calculations, γ evolves monotonously and continuously through the Lifshitz transition (Fig. 2b of Ref. [7]). (In other heavy-fermion settings, experiments have implicated a Zeeman-induced Lifshitz transition at a high field [9, 10], with the effective mass *decreasing* on approach of the transition.) This is in drastic contrast to the experiments in YbRh₂Si₂: both the enhancement and divergence of the effective mass have been observed. This divergence is most clearly inferred from the resistivity A -coefficient on both sides of the critical field [6]. It has also been observed through the measurement of the specific-heat coefficient γ on the elevated-field side [6], and is consistent with the behavior of the measured γ in the low-field regime [11].

We close by noting that the most striking feature of the phase diagram of YbRh₂Si₂ is that the $B^*(T)$ line terminates at the AF phase boundary as $T \rightarrow 0$, *i.e.* the AF critical B_N equals $B^*(T = 0)$, as shown in Fig. 1b (Ref. [1]), and there is evidence that this property extends to a range of finite (negative) chemical pressure as seen in Fig. 2 (Ref. [12]). It is hard to imagine how

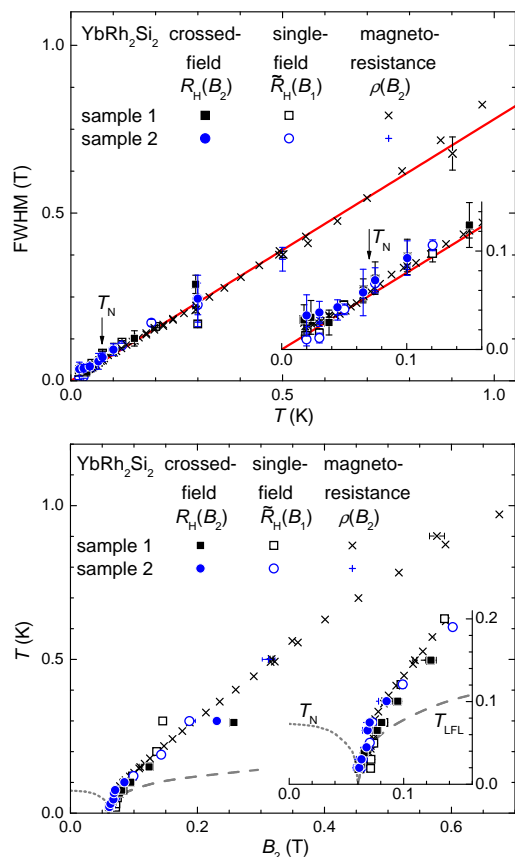


FIG. 1: (a) Full width at half maximum (FWHM, Γ) of the crossovers in the Hall coefficient and magnetoresistivity. The solid line represents a linear fit to all data sets. Within the error this line intersects the origin. The inset magnifies data at the lowest temperatures. The arrow indicates the Néel temperature at $B = 0$; (b) Position of the crossover fields in the temperature–magnetic field phase diagram, $B^*(T)$, as determined from measurements of the Hall coefficient and longitudinal magnetoresistivity. The inset magnifies the low temperature range. The dotted and dashed lines respectively represent the Néel temperature and the crossover to low- T Landau Fermi-liquid (LFL) behavior on the paramagnetic side, as deduced from resistivity measurements. (From Ref. [1].)

this could emerge out of a fine-tuned bandstructure of non-interacting electrons with no connection to the AF transition.

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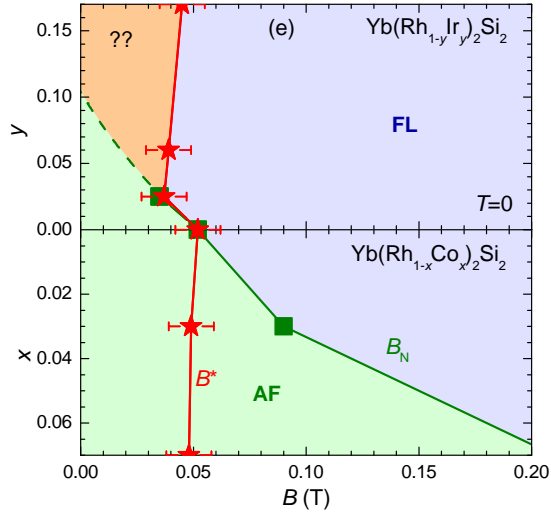


FIG. 2: Zero-temperature phase diagram of $\text{Yb}(\text{Rh}_{1-x}\text{M}_x)_2\text{Si}_2$ ($M = \text{Ir}, \text{Co}$). B^* and B_N are respectively the low-temperature limit of the crossover field and the field for the AF transition; their variations with composition are depicted. Green and blue shaded region mark the AF ordered and paramagnetic Fermi-liquid ground state, respectively. (From Ref. [12].)

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